

Varian NMR Manual

Standard Operation Training Course

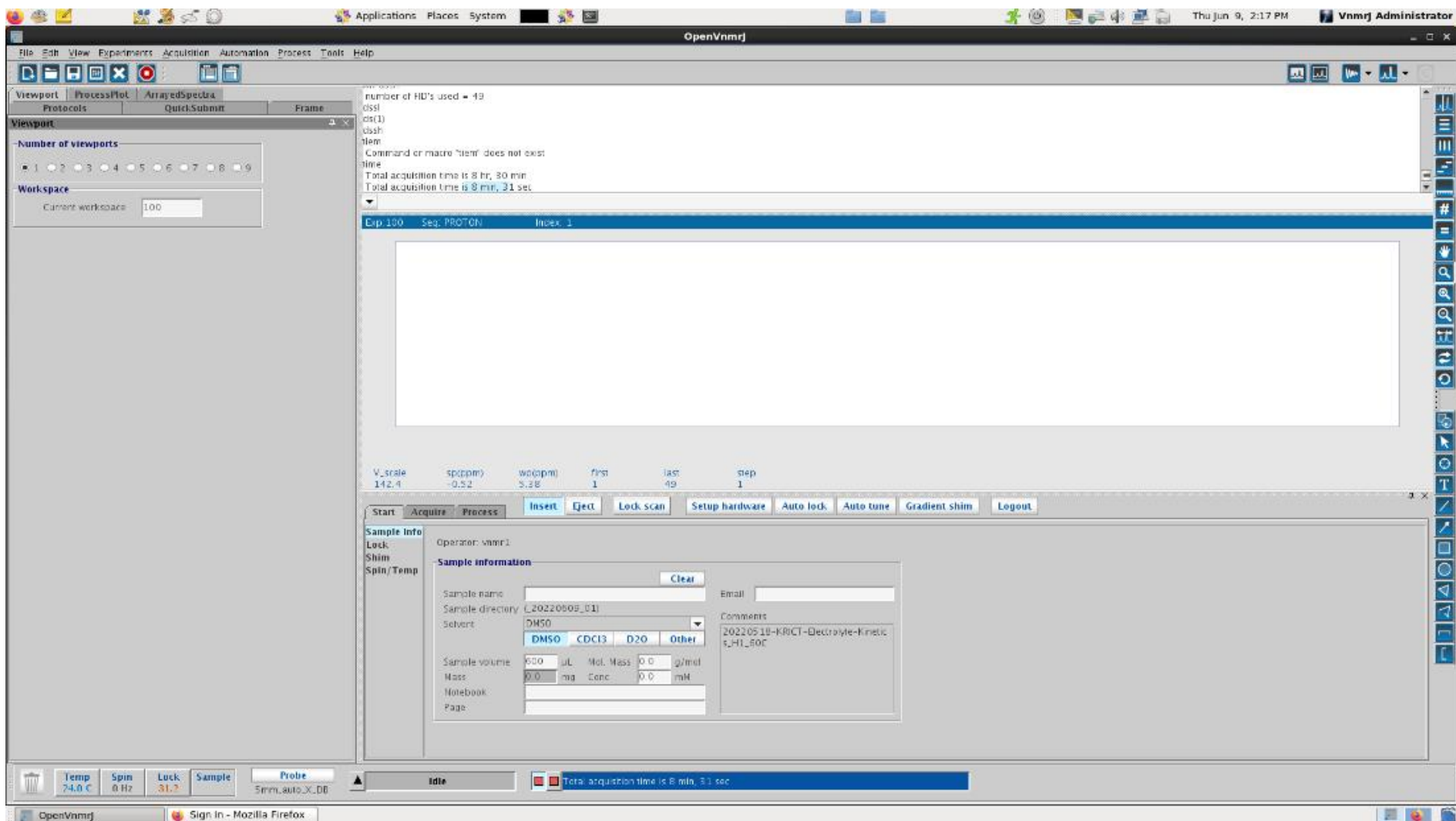


1. Software

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OpenVnmrJ 2.1A in CentOS 6.10



<https://github.com/OpenVnmrJ/OpenVnmrJ/blob/master/Install.md>

OpenVnmrJ 3.1A

CentOS: Versions 7.5, 7.6, 7.7, 7.8, 7.9

RHEL: Versions 8.4

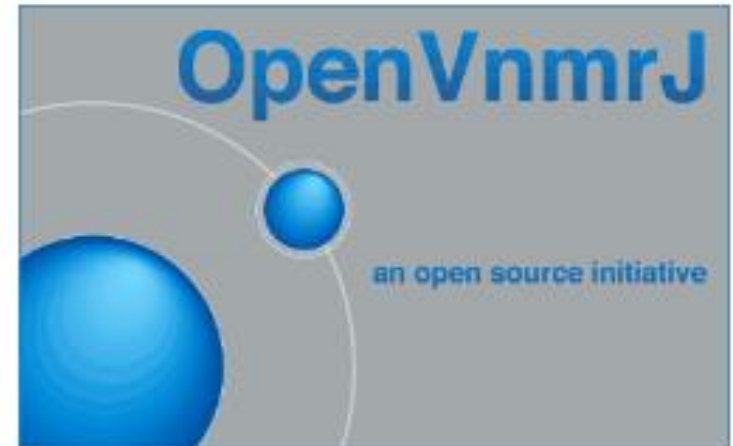
AlmaLinux: Version 8.4

Ubuntu: Version 20.

OpenVnmrJ 2.1A

RHEL/CentOS: Versions 6.8, 6.9, and 6.10

RHEL/CentOS: Versions 7.5, 7.6, 7.7, 8.1, and 8.2



2. Quick Guide

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2-1. Automation

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Automation

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Viewport ProcessPlot ArrayedSpectra

Protocols QuickSubmit Frame

Experiment Selector

Solids Experiments Tests AutoSolids Experiments

Common Liquids Calibration Service

PROTON	CARBON
(H)PRESAT	(H)wet1D
(HH)gCOSY	(HC)HSQCAD
(HC)gHMBCAD	(H)NOESY1D
Studies ▾	

Study Queue

☐ Sample ☐ Active sample ☒ Spectrometer ☐ Study cluster Options

auto_20220106_01

2

New study Continue study

Temp 24.0 C Spin 0 Hz Lock 43.8 Sample Probe 5mm_auto_X_DB

Viewport ProcessPlot ArrayedSpectra

Protocols QuickSubmit Frame

Experiment Selector

Solids Experiments Tests AutoSolids Experiments

Common Liquids Calibration Service

PROTON	CARBON
(H)PRESAT	(H)wet1D
(HH)gCOSY	(HC)HSQCAD
(HC)gHMBCAD	(H)NOESY1D
Studies ▾	

Study Queue

Submit queue Cancel

New Sample

SampleInfo [0:00]

New study Submit to Background ▾

Clear pending exp from queue

Viewport ProcessPlot ArrayedSpectra

Protocols QuickSubmit Frame

Experiment Selector

Solids Experiments Tests AutoSolids Experiments

Common Liquids Calibration Service

PROTON	CARBON
(H)PRESAT	(H)wet1D
(HH)gCOSY	(HC)HSQCAD
(HC)gHMBCAD	(H)NOESY1D
Studies ▾	

Study Queue

Submit queue Cancel

New Sample

SampleInfo [1:24]
PROTON_001 [0:24]

New study Submit to Background ▾

Clear pending exp from queue

Temp 24.0 C Spin 0 Hz Lock 43.8 Sample Probe 5mm_auto_X_DB

Automation

Viewport ProcessPlot ArrayedSpectra

SampleInfo [1:24]
PROTON_001 [0:24]

DATA
Labs
Automation
Solid_state_NMR

New Sample
SampleInfo [1:24]
PROTON_001 [0:24]

Submit

Temp 24.0 C Spin 0 Hz Lock 43.8 Sample Probe 5mm_auto_X_DB

Sample_name (to be submitted)
SampleInfo [1:24]
PROTON_001 [0:24]

Acquire Process Insert Eject Logout

Operator : vnmr1

Sample information

Sample name Sample_name

Sample directory Sample_name_20220603_001

Solvent CDCI3
DMSO CDCI3 D2O Other

Sample volume 600 µL Mol. Mass 0.0 g/mol
Mass 0.0 mg Conc. 0.0 mM

Notebook
Page

Study time: 1 min, 24 sec

Save

Acquisition options

Spectral width (select) -2.0 to 14.0 ppm
(...or enter)

Number of scans 8
Relaxation delay 1 s
Pulse angle 45 degrees
Minimize SW Skip
Calibrate pw90

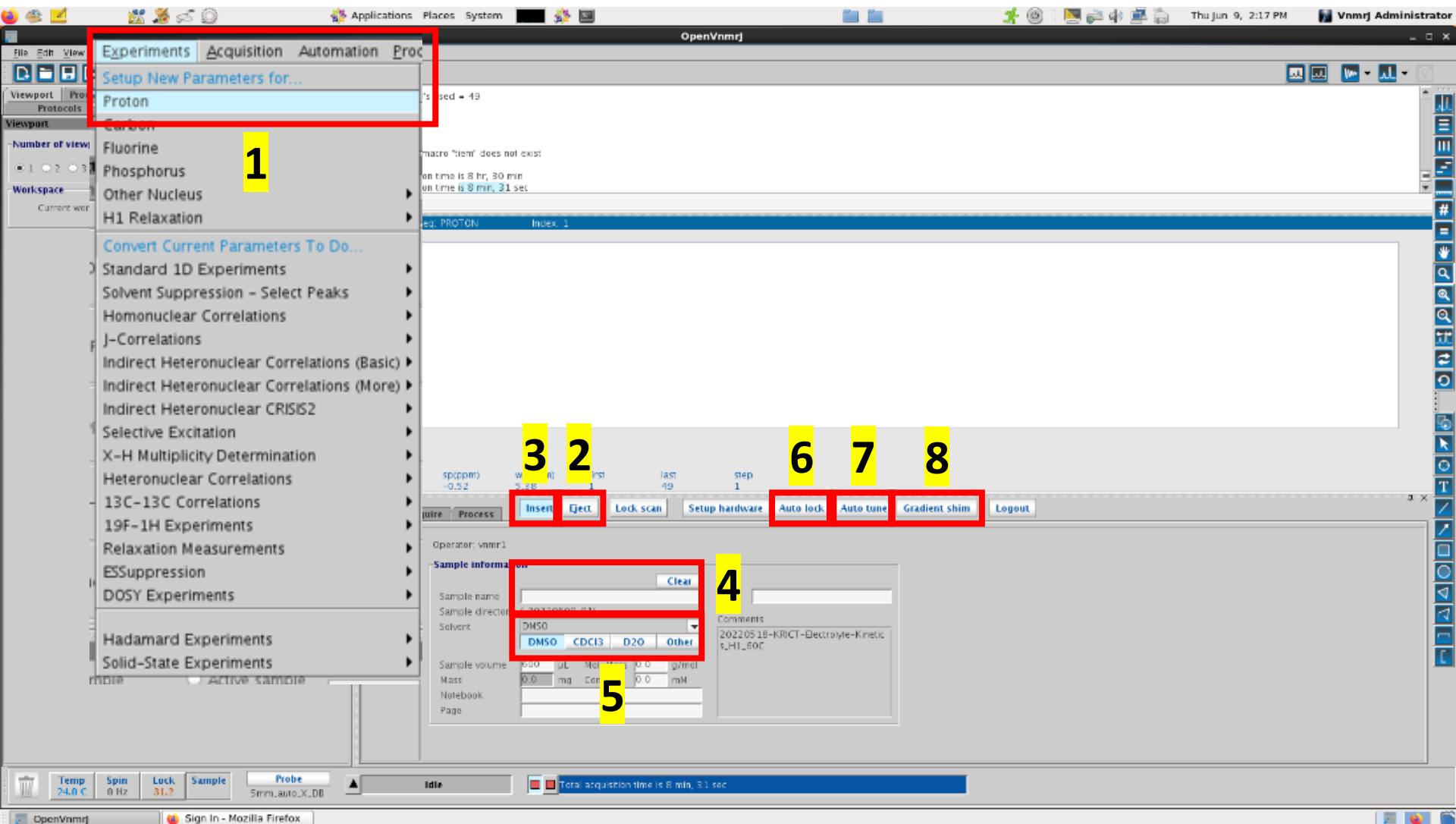
Adding PROTON to queue

2-2. Manually operation

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Choice experiments



Choice experiments

The screenshot displays the Bruker Vnmrj software interface with several key components highlighted by numbered annotations:

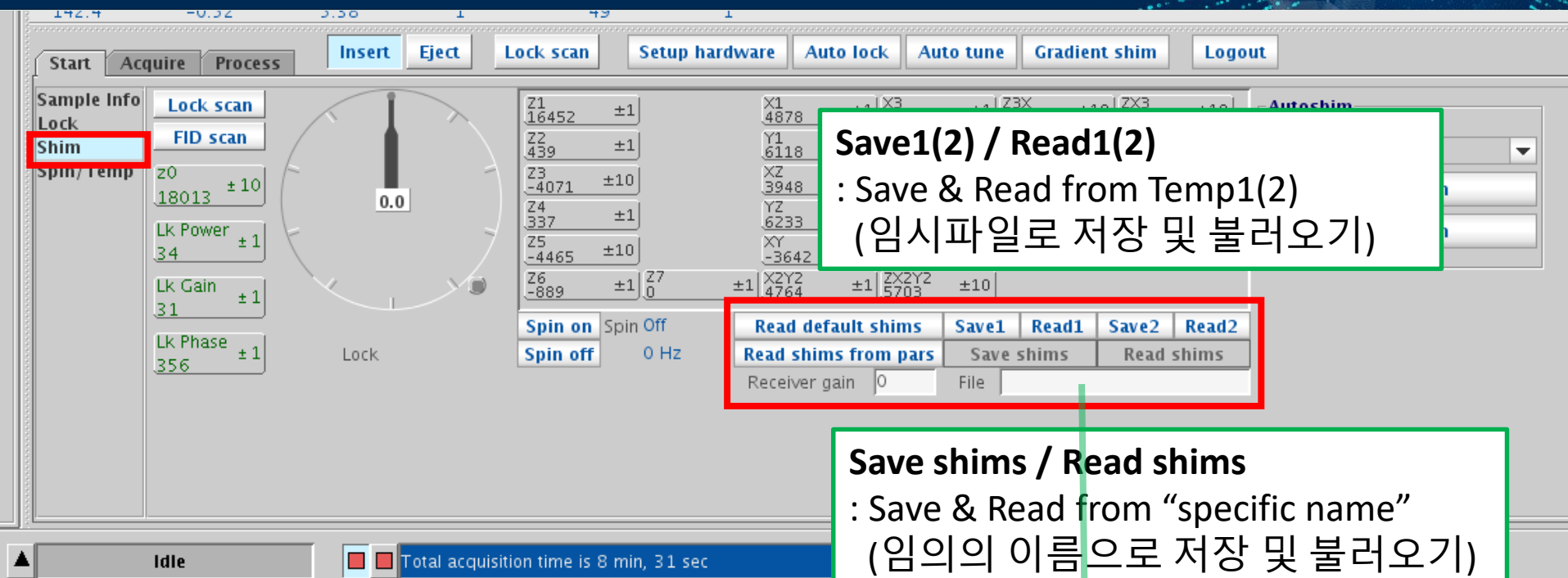
- Top Bar:** Contains buttons for **Start**, **Acquire**, **Process**, **Insert** (3), **Eject** (2), **Lock scan**, **Setup hardware**, **Auto lock** (6), **Auto tune** (7), **Gradient shim** (8), and **Logout**.
- Sample Info Panel:** Includes checkboxes for **Spin** and **Lock**, a **Lock status** indicator, and buttons for **Select lock signal...** and **Find z0**. A green box labeled **Change sample** is positioned over the **Lock** checkbox area.
- Lock Parameters:** A table showing lock parameters: **Gain** (34, ±1), **Phase** (31, ±1), and **356**.
- Autolock Panel:** Features radio buttons for **Automatic**, **Sample**, **z0 only**, **Unlocked**, and **Not used**, along with a **Run autolock** button.
- Bottom Bar:** Includes buttons for **Show time**, **Go** (12), **Stop**, **MoveSW**, **Est. pw90**, **Arrays**, **Sequence diagram**, and **Help** (14).
- Left Panel:** Contains a sidebar with **Default H1** (10) and **Acquisition options** (11). The **Acquisition options** section includes a table for **Spectral width (select)** (-2.0 to 14.0 ppm), **Number of scans** (8), **Relaxation delay** (1 s), and **Pulse angle** (45 degrees).
- Right Panel:** A file explorer showing a directory structure with **DATA**, **Labs**, **Automation**, and **Solid_state_NMR** folders. A red box highlights the **DATA** and **Labs** folders.
- File Menu:** A dropdown menu is open, showing options like **New Workspace**, **Join a New Workspace**, **Open...** (Ctrl-O), **Save As...** (Ctrl-S), **Auto Save**, **Printers...**, **Print Screen...**, **Auto Plot**, **Review PDF Plots...**, **Switch Operators...**, and **Exit Vnmrj**. A red box highlights the **Save As...** option.

3-1. Start tab

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Start - Shim



Read default shims

: Read shim from Gradient shim-map
(Gradient shim-map을 가져옴)

Read shims from pars

: Read shim from experiments
(실험방에서 shim-map을 가져옴)

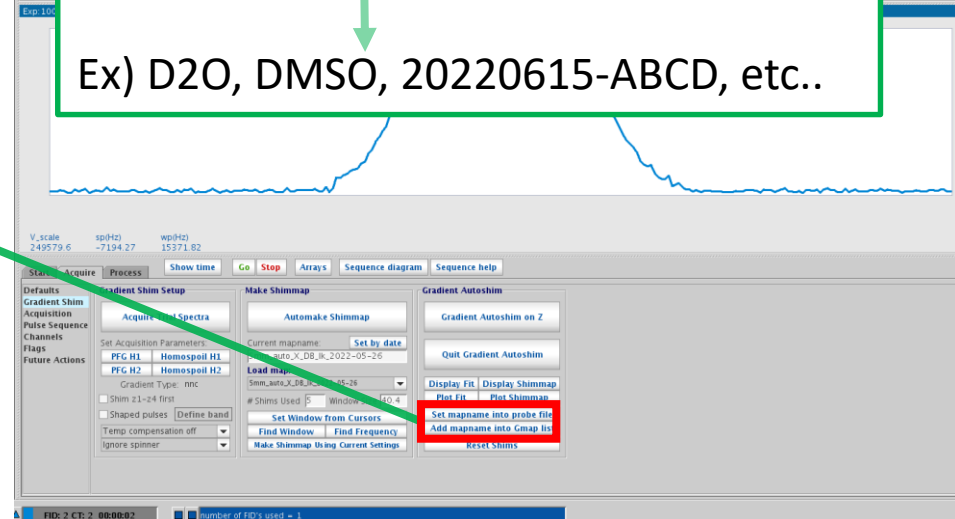
Save1(2) / Read1(2)

: Save & Read from Temp1(2)
(임시파일로 저장 및 불러오기)

Save shims / Read shims

: Save & Read from "specific name"
(임의의 이름으로 저장 및 불러오기)

Ex) D2O, DMSO, 20220615-ABCD, etc..



Start – Spin

Start Acquire Process Insert Eject Lock scan Auto tune Gradient shim Logout

Sample Info Lock Shim

Spinner: liquids

Regulate speed

0 [Slider] 100

Current 0 Hz Off Spin off

Spin
Type 20
Enter
Click Regulate speed

Temperature

Regulate temp

60 [Slider] 100

Current 24.0 C Regulated FTS 0.0 C

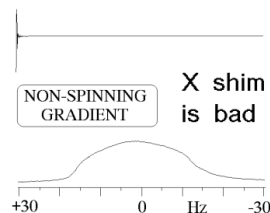
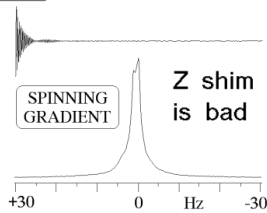
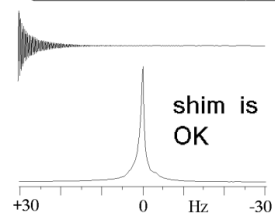
VT air flow 2 l/min VT air on VT air off

Reset pneumatics Reset VT Set FTS temp 25

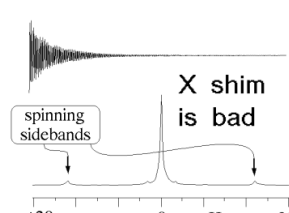
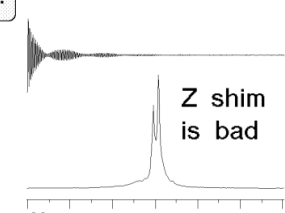
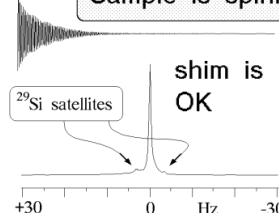
Warn after temperature error
Ignore temperature error

Idle Total acquisition time is 8 min, 31 sec

Sample is NOT spinning.



Sample is spinning.



https://medicine.uiowa.edu/nmr/sites/medicine.uiowa.edu.nmr/files/wysiwyg_uploads/Shimming%20an%20NMR%20Magnet.pdf

Start – Temp

Start Acquire

Sample Info Lock Shim Spin/Temp

Temperature
Type 50 (target temp)
Enter
Click

Regulate temp Temp off

60

Current 24.0 C Regulated FTS 0.0 C

VT air flow 2 l / min VT air on VT air off

VT air flow -> 6 °C / min
Extreme temperature change
could break Quartz in Probe.

Sensor Thermocouple Pt-100

VT flow cause Temp. gradient.
Stabilization time: 5 – 15 min

Heater

VT Unit

The image shows a screenshot of the NMR control software interface. On the left, there are tabs for 'Start', 'Acquire', 'Sample Info', 'Lock', 'Shim', and 'Spin/Temp'. The 'Spin/Temp' tab is selected. Below the tabs, there is a 'Temperature' section with a 'Regulate temp' button and a 'Temp off' button. A slider is set to 60. Below the slider, it shows 'Current 24.0 C', 'Regulated', and 'FTS 0.0 C'. At the bottom of the temperature section, it shows 'VT air flow 2 l / min' and buttons for 'VT air on' and 'VT air off'. A green box highlights the 'Temperature' section. Another green box highlights the 'VT air flow' section with the text 'VT air flow -> 6 °C / min' and 'Extreme temperature change could break Quartz in Probe.' On the right, there is a diagram of the probe assembly. It shows a vertical tube with a 'Sensor Thermocouple Pt-100' at the top. A 'Heater' is located at the bottom of the tube. A 'VT Unit' is connected to the heater. A green box highlights the diagram with the text 'VT flow cause Temp. gradient. Stabilization time: 5 – 15 min'.

3-2. Acquire tab

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Acquire tab

Start **Acquire** Process Show time Go Stop MoveSW Est. pw90 Arrays Sequence diag

Default H1 **Acquisition** Pulse Sequence Channels Flags Future Actions Overview

PROTON

Spectrum width (SW)

Spectral width 9615.4
Acquisition time 1.704
Complex points 16384

Excitation

Relaxation delay 1.000 s
First pulse 0.00 μs
Inter-pulse delay 0.000 s
Observe pulse 5.00 μs
Calibration pw90 10.00 μs at power 62 dB

Scans

Requested 8
Completed 0
☐ Steady state 0
☒ Block size 32

Receiver

Receiver gain 38
Timing (μs) rof2 24.81

Annotations:

- aq (AQ)
- TD
- D1 (D1)
- pw (P1)
- nt (NS)
- ss (DS)
- bs (type tr)
- tpwr (plw1)
- Type rga

Start Acquire **Process** Show time Go Stop MoveSW Est. pw90 Arrays Sequence diagram Sequence help

Default H1 **Channels** Pulse Sequence Flags Future Actions Overview

PROTON

Channels: Observe set 1 Decouple set 2 Decouple 3

Nucleus / freq. H1 599.826 MHz C13 150.840 MHz 0.000 MHz

Offset 599.80 Hz 0.00 Hz 0.00 Hz

Dec on/off
Dec modula
90 deg. at pwr 10.00 μs at 62 28.5 μs at 39 31.0 μs at 1
= dmf Homodec --- = 35088 = 32258
Waveform --- W40_5mm_auto_X_DB
at resolution --- degrees 9.00 degrees 1.00 degrees

Annotations:

- Spectrum center (O1)

Acquire tab

Start Acquire Process Show time Go Stop MoveSW Est. pw90 Arrays Sequence diagram Sequence help

Default H1 Acquisition Pulse Sequence Channels **Flags** Future Actions Overview

Flags

On lock failure Ignore On VT failure On spin failure

Allow 300 s before VT testing Do not wait for temp or spin

Delay 0.5 s before starting acquisition

☒ Save FID at each block Block size 32

☐ Acquire arrays by blocks (interleave) ☒ 32-bit acquisition (normal)

Receiver

Receiver gain 38 Auto Pulse sequence type Pulse

Timing (μs) rof2 24.8 alfa 10.0 ddrtc 37.20

Prescan delay

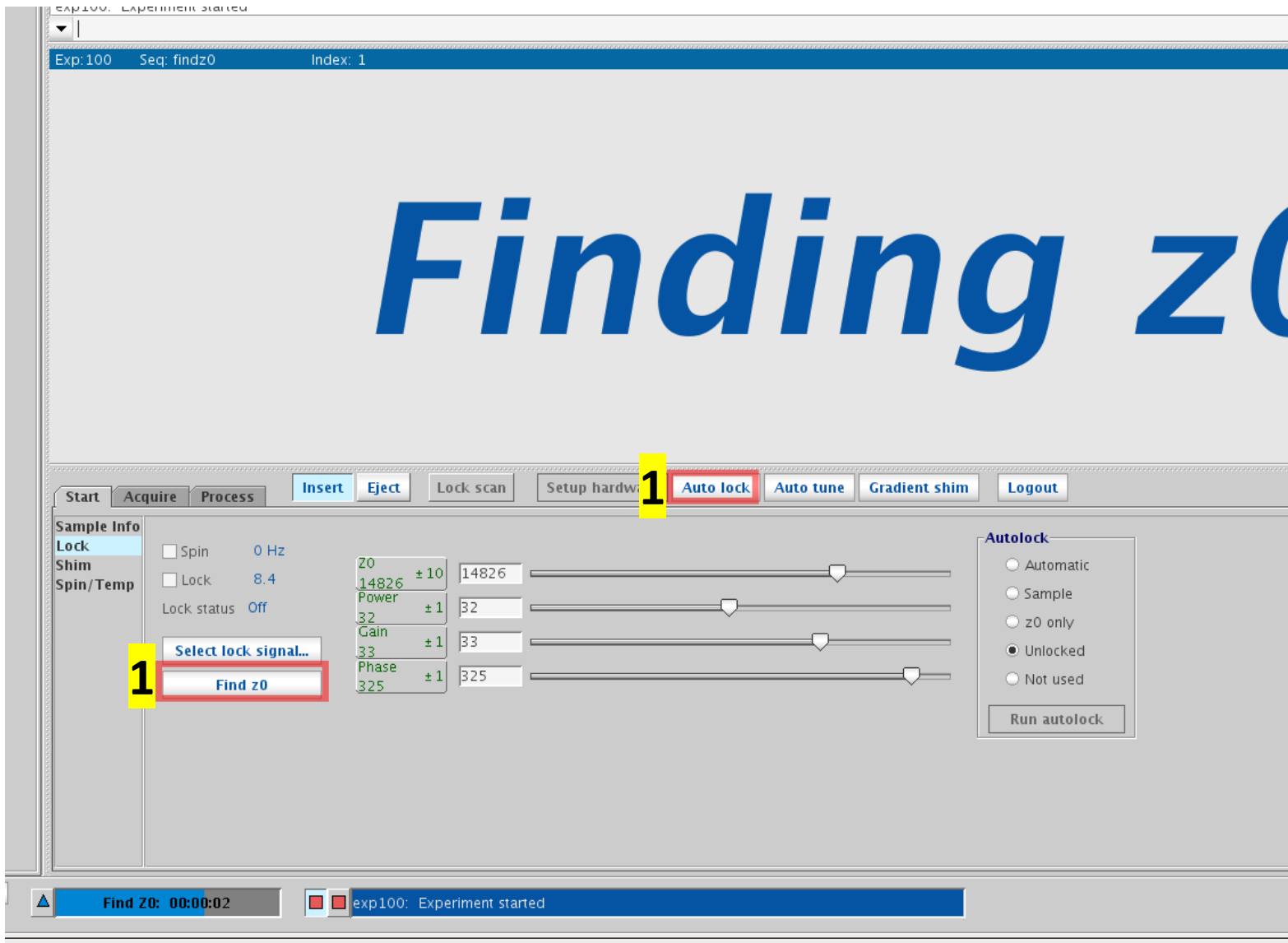
Idle exp100: Acquisition complete

4-1. Lock

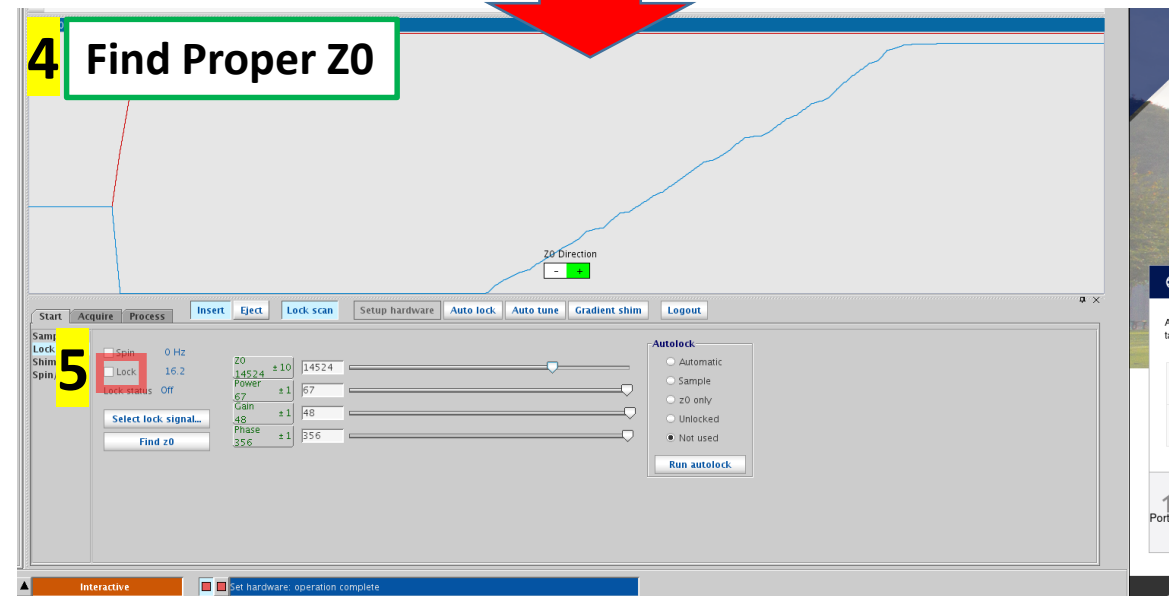
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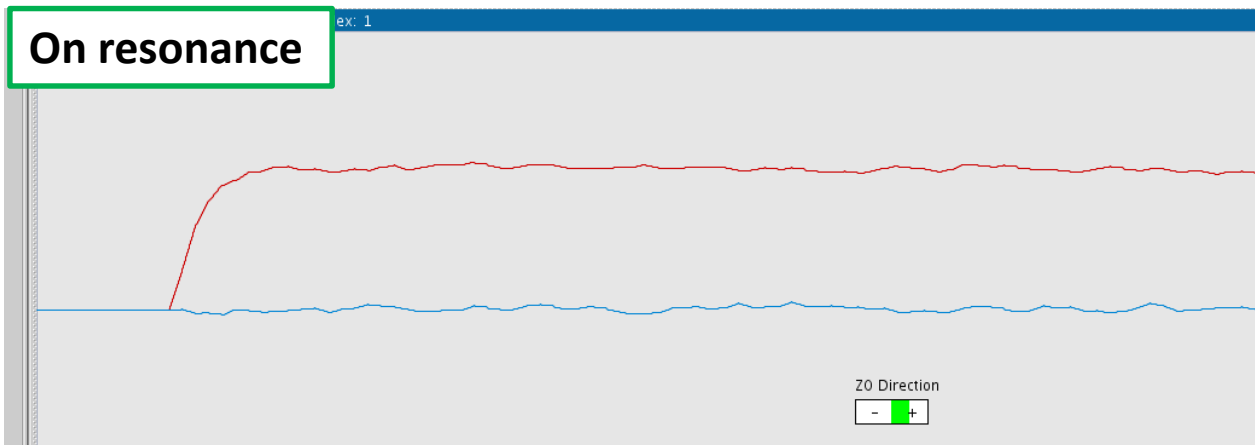
Lock (Auto)



Lock (Manual)



Lock (Manual)



4-2. Tune & Match

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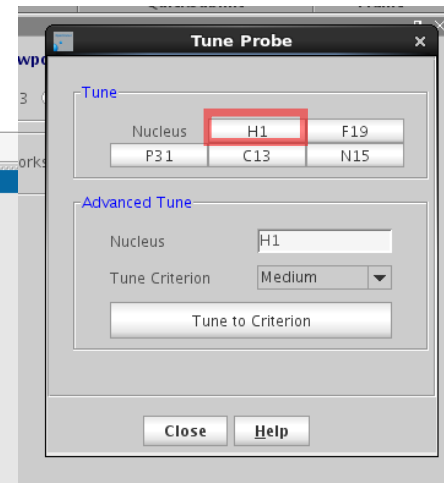
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Tuning and Matching

Tune method

1. Click Auto tune
2. Type protune on command line
3. Type protune('calibrate') on command line
4. Probe -> Tune sweep -> Manual tune

2. Type protune



1. Click Auto tune

Start Acquire Process Insert Eject Lock scan Setup hardware Auto lock **Auto tune** Gradient shim Logout

Sample Info
Lock
Shim
Spin/Temp

☐ Spin 0 Hz
☐ Lock 0.1
Lock status Off

Select lock signal...

Find z0

Z0 17927 ±10
Power ±1
28 Gain ±1
31 Phase ±1
360

17927
28
31
360

Autolock

- ☐ Automatic
☐ Sample
☐ z0 only
☐ Unlocked
☒ Not used

Run autolock

New study

Continue study

4. Probe -> Tune sweep -> Manual tune

Probe

5mm_auto_X_DB

Idle

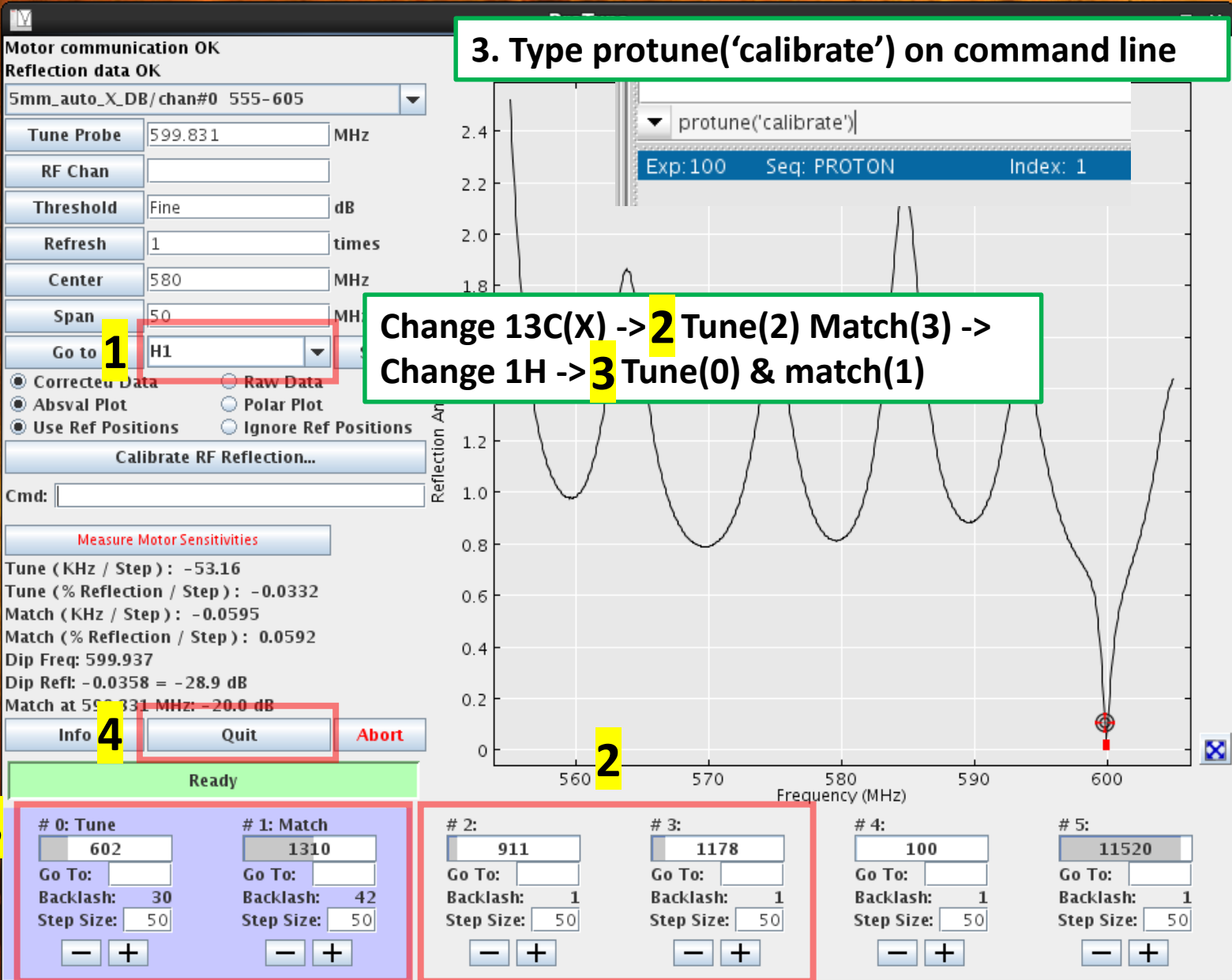
Set hardware: operation complete

Protune (manual)

3. Type protune('calibrate') on command line

Change 13C(X) -> **2** Tune(2) Match(3) ->
Change 1H -> **3** Tune(0) & match(1)

3



Tune sweep

1 **Probe**

2 **Tune Sweep**

3 **Tune RF channel**

4 **Start Probe Tune**

5 **Manually control tune stick**

Current probe: 5mm_auto_X_DB

Edit/Show Probe file

Tune Gain: 0

Default Shims: 5mm_auto_X_DB_1k_d2o

Load Shims

Manage probe files

Edit/Show/Delete:

5mm_auto_X_DB (Home)

Edit Show Delete

Create/Copy:

Probe name:

Probe ID: Probe without ID

Probe style:

ApplicationsDir: Home account

Create Copy

Close Help

Options

Sample Active sample Spectrometer Study cluster

auto_20220106_01

New study Continue study

Temp 24.0 C Spin 2 Hz Lock 43.8

Probe

Probe Tuning

Tuning done: ok

OpenVnmrj

Exp: 100 Seq: mtune Index: 1 mouse: [LEFT] click to set first cursor [RIGHT] click to set second cursor [MIDDLE] click or scroll to scale

H1

5

8000 7000 6000 5000 4000 3000 2000 1000

MHz

V_position 0 V_scale 1.8 cursor 301.49 delta 4.03

Start Acquire Process Insert Eject Lock scan Setup hardware Auto lock Auto tune Gradient shim Logout

Probe

Tune RF channel 1

Center Frequency H1 H1 Freq 599.83 M Span 10.0 M

Choose Marker 1 Choose Marker 2

Center frequency to markers

Power 0 dB Gain 0 dB

Vertical scale *2 /2 Autoscale # Points 512

Vertical position +20 -20

Start Probe Tune Stop Probe Tune Quit

4-3. Processing

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Type wft

1 **2**

Exp: 100 Seq: PROTON Index: 1

5.69

ppm

V_position 33.0 V_scale 55141.1 cursor 9.57 delta

Start Acquire **Process** **Transform** Auto process Display spectrum Auto plot preview Clear screen Cancel

Sample information

Sample:
Solvent: dmso
Sample owner: vnmr1

Comments: 20220520-TM200-2015j6111_H1

Process options

FT data size: 64k
☒ LineBroaden: 0.6 Hz

Plot options

Parameters: Basic
Integrals: Off
Peak Values: Peaks ppm

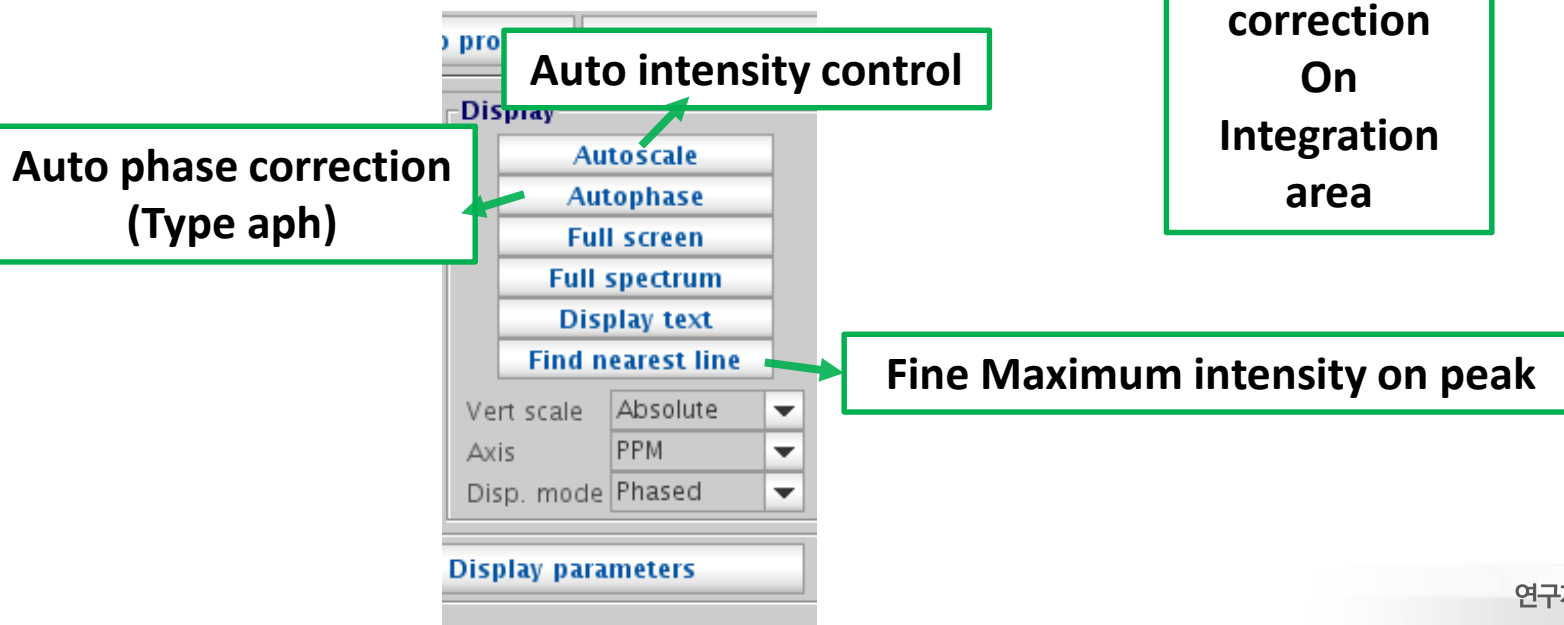
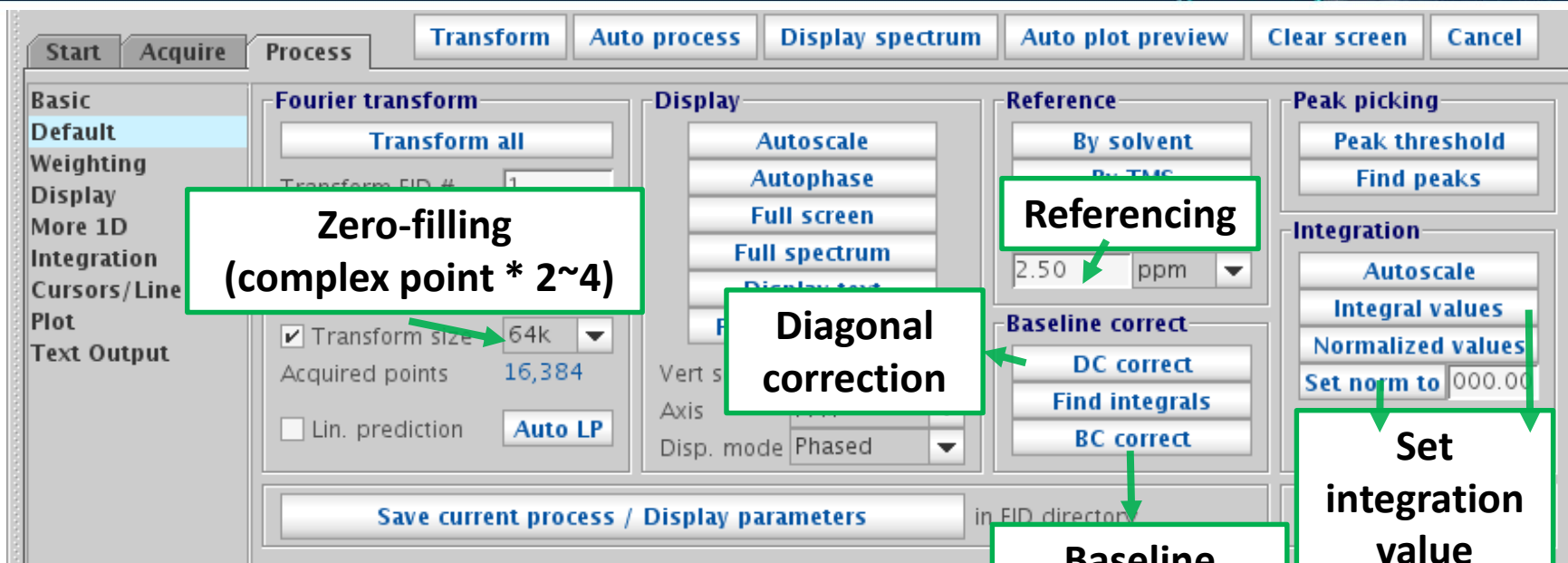
Process Auto plot Auto preview

Display spectrum Save current process/display parameters

Temp 24.0 C Spin 0 Hz Lock 31.3 Sample Probe 5mm_auto_X_DB

FID: 1 CT: 2 00:01:53 processing: /home/vnmr1/Desktop/DATA/ENF/QC/20220520-TM200-2015j6111_H1.fid

Process tab



Process tab

Start Acquire **Process** Transform Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic
Default
Weighting
Display
More 1D
Integration
Cursors/Line Lists
Plot
Text Output

Fourier transform

Transform all ☒ Transform size 64k
Transform FID # 1 Acquired points 16,384

AutoSelect weighting

exponential	gaussian
sine	cosine
sq-sine	sq-cosine
pseudo	res-enhance
/4 ssqsine	

Weight parameters

line broadening	0.6	☒
sinebell	0	☐
shift	0	☐
gaussian	0.1	☐
shift	0	☐
additive offset	0	☐

Zero-filling
(Complex point * 2~4)

Line broadening (LB)
1H: 0.6 - 1
13C: 3

Linear Prediction (LP)
: 2 ~ 3 (Case by case)

Start Acquire **Process** Transform Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic
Default
Weighting
Display
More 1D
Integration
Cursors/Line Lists
Plot
Text Output

Linear prediction

☒ LP ON/OFF **Auto**
☒ Back ☐ Forward

Coefficients 32
Basis points 64
starting at 2
Predicted points 1
starting at 1

Acquired points 16,384
☒ FT size 64k
Weighting exponential

Downsample

☐ Downsampling ON/OFF
Divide by ---
Coefficients ---
Offset ---

☐ FID phase rotation 0.0 degrees
☐ Left shift FID 0 complex points
☐ Left shift frequency 0 Hz

Cut off FID signal for Aring (ringing)
ex) Short T1 experiments_17O, 23Na,
79Br, 127I, etc..)

Process tab

Start Acquire **Process** Transform Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic Spectral graphics

Show integration line or not

Integration
Cursors/Line Lists
Plot
Text Output

Logo
☐ None ☒ Custom [Browse...](#)

☐ Integral lines
☐ Full ☐ Partial
☒ Integral values
☒ Scaled ☐ Normalized
☐ Horiz ☒ Vert

Peak labels
 ppm
☒ Axis
☒ ppm ☐ Hz
☐ Molecule

Lists

Parameters
☐ Basic ☒ All ☐ None

Integral values
☒ Integral list
☒ Scaled ☐ Normalized

Peak positions
☒ Peak list
☒ ppm ☐ Hz

☒ Comments ☒ Miniplots

Send to
 Hz per mm: 28.2
☐ Print 1 page
☐ Print 2 pages
☒ Print double-sided

[Preview](#) [Print](#)

Show PDF

Start Acquire Process **Transform** Auto process Display spectrum Auto plot preview Clear screen Cancel

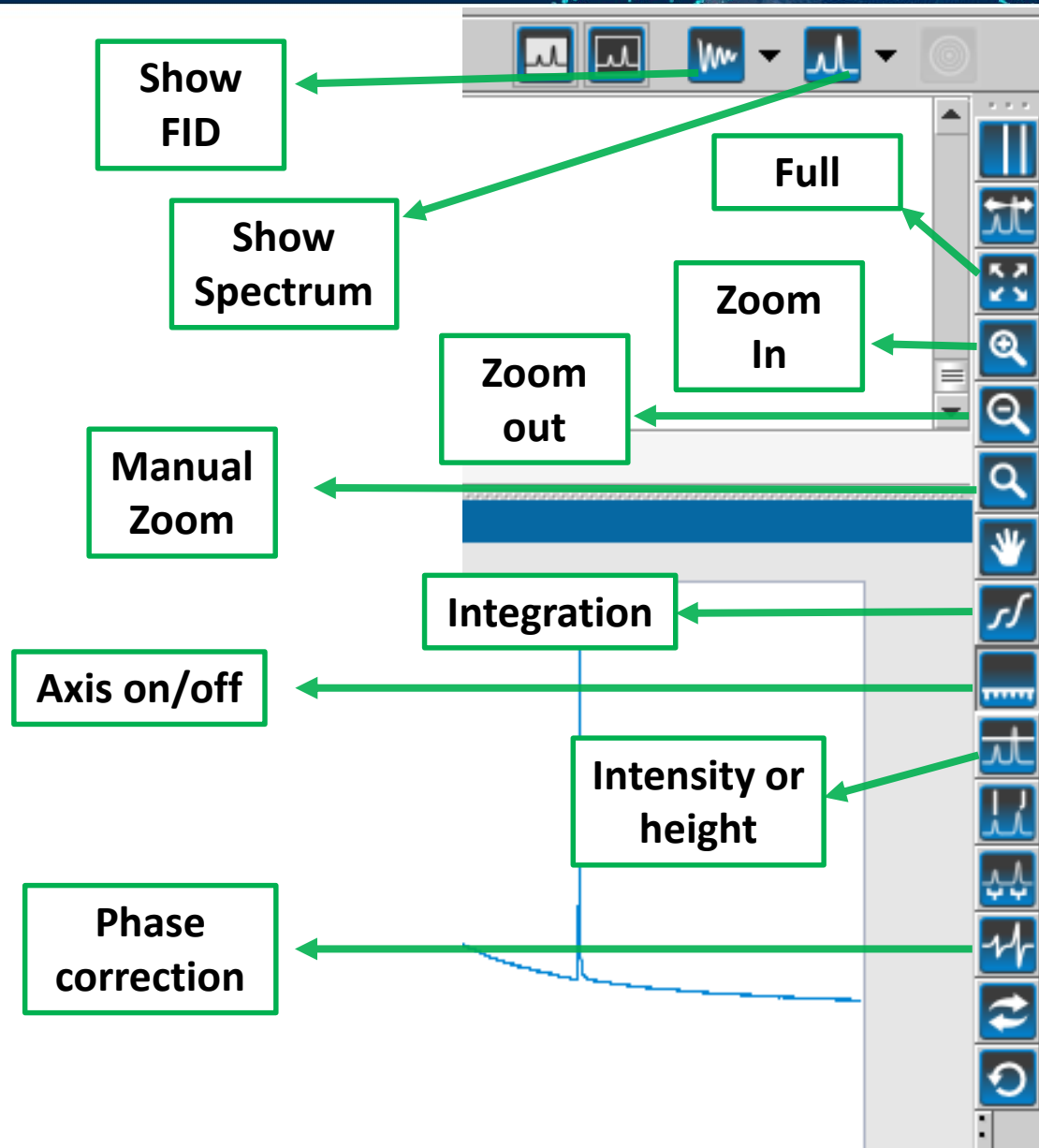
Basic
Default
Weighting
Display
More 1D
Integration
Cursors/Line Lists
Plot
Text Output

ACQUISITION		SAMPLE		PROCESSING		GRADIENT SHIM	
sfrq	92.077	date	Jun 16 2022	fn	not used	gzsize	5
tn	1k	file	/home/vnmr1/v~	sb	not used	gzlvl	2000
at	0.017	nrmr	sys/gshimlib/sh~			gzwin	30.3
np	512	immr	aps/5mm_auto_X_~	wnt	wft f vsadj ds~	d2	0.0010
sw	15432.1	DB	1k_2022-06-16-A~	sh		d3	arrayed
ss	1	.fid				vtcomplv1	0
tpwr	45	solvent	D2O			gstab	0.00025
pw	300.0	temp	24.0			shift	0.00300
d1	3.000						
tof	15.1	DECOUPLING					
nt	4	dn	H1				
ct	4	dof	0				
gain	26	dm	n				
		dmm	c				
		dmf	200				
		dpwr	30				

FLAGS

Show Manual

Text
Basic
Array
Channels
Shims
Seq manual
More
Clear



5-1. Maintenance

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Affecting factors for Shimming

1. Temperature and Temperature gradient
2. Tube (Camber, Thickness, Scratch, Material quality, Impurity contents)
3. Height
4. Sample (Concentration, Paramagnetic species, Impurity, Ion/salt, Particle)
5. Solvent (Viscosity, Dielectric constant)

Axial shims(on axis): Z1, Z2, Z3, Z4, Z5, Z6, etc..

Radial shims(off axis): X, Y, XY, XZ, YZ, X2Y2, etc..

Ex) $X = X + Z0$, $XZ = X + Z1$

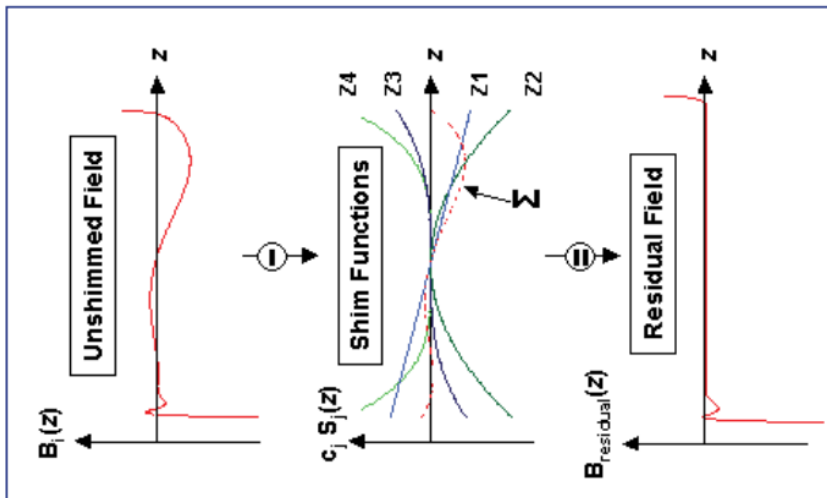
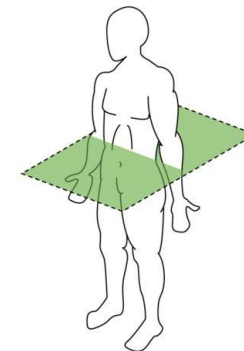
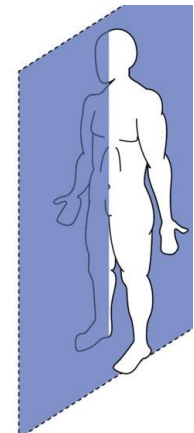


Fig. 7: The 1D gradient shimming algorithm. In a one-time calibration experiment it is necessary to use the method of Fig. 5 to measure the actual

Transverse plane
(Radial)
X, Y shims



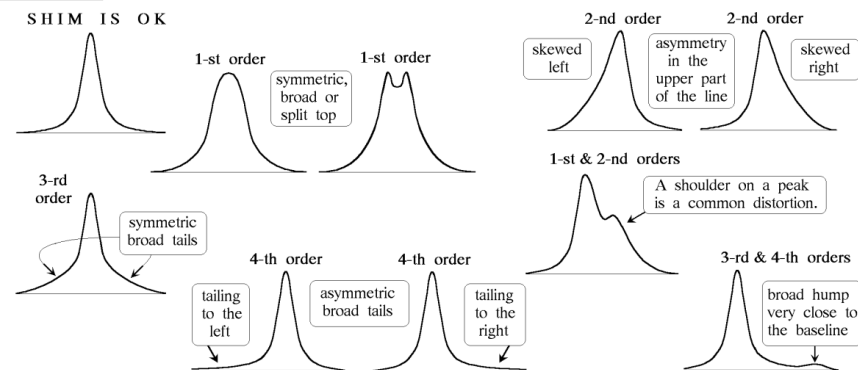
Longitudinal plane
(Axial)
Z shims



Class of shim coil

SHIM CONTROLS ON THE SPECTROMETERS					spinning/ non-spin	high/ low	odd/ even	order
FX-90Q	WM-360	MSL-300	AC-300	AMX-600				
Y	Z	Z	Z	Z	spinning	low	odd	1-st
C	Z ²	Z ²	Z ²	Z ²	spinning	low	even	2-nd
Y ³	Z ³	Z ³	Z ³ Z ⁵	Z ³ Z ⁵	spinning spinning	high high	odd odd	3-rd 5-th
F	Z ⁴	Z ⁴	Z ⁴	Z ⁴	spinning	high	even	4-th
Z X	X Y	X Y	X Y	X Y	non-spin non-spin	low low	odd odd	1-st 1-st
ZX XY YZ X ² -Y ²	XY YZ XZ X ² -Y ²	XY YZ XZ X ² -Y ²	XY YZ XZ X ² -Y ²	XY YZ XZ X ² -Y ²	non-spin non-spin non-spin non-spin non-spin	low low low low low	even even even even even	2-nd 2-nd 2-nd 2-nd 2-nd
X ³ Z ³	X ³ Y ³	X ³ Y ³ XZ ² YZ ²	X ³ Y ³ XZ ² YZ ²	X ³ Y ³ XZ ² YZ ² ZXY Z(X ² -Y ²)	non-spin non-spin non-spin non-spin non-spin non-spin non-spin	high high high high high high high	odd odd odd odd odd odd odd	3-rd 3-rd 3-rd 3-rd 3-rd 3-rd 3-rd
				XZ ³ YZ ³	non-spin non-spin	high high	even even	4-th 4-th
Y	Z				<--- spinning axis for NMR tubes			

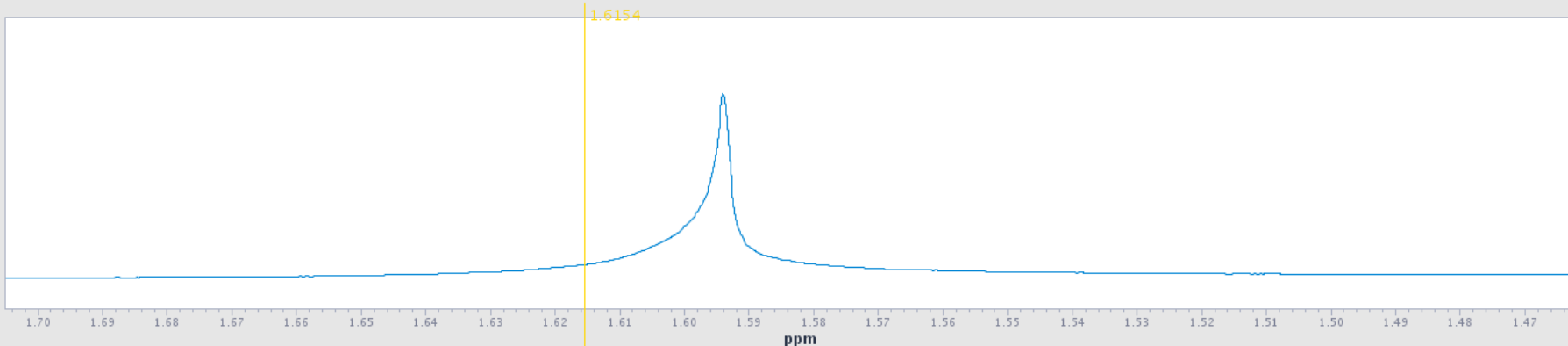
Doped 1% H₂O in D₂O
Bruker 400 MHz linewidth 4 Hz
Varian 600 MHz linewidth 6 Hz



SKETCHES OF LINE DISTORTIONS CAUSED BY VARIOUS GRADIENTS

Manual shim

Exp: 100 Seq: PROTON Index: 1 mouse: [LEFT] click to set first cursor [RIGHT] click to set second cursor [MIDDLE] click or scroll to scale



V_position 13.6
V_scale 5419.8
cursor 1.4617

Shim value +/- 32767

Start 2 Acquire Process Insert Eject Lock scan Setup hardware Auto lock Auto tune Gradient shim Logout

Sample In Lock scan
Shim 3 FID scan
Spin/T 3 Spectrum
4 Disp Linesh
DC correct
Autophase

6

Z1 16452 ±1	X1 4878 ±1	X3 -877 ±1	Z3X -467 ±10	ZX3 -6623 ±10
Z2 439 ±1	Y1 6118 ±1	Y3 125 ±1	Z3Y 4666 ±10	ZY3 -6320 ±10
Z3 -4071 ±10	XZ 3948 ±1	XZ2 6225 ±1	Z2XZ2 -3089 ±10	Z4X 4174 ±10
Z4 337 ±1	YZ 6233 ±1	YZ2 11877 ±10	Z2XY -2404 ±10	Z4Y -4745 ±10
Z5 -4465 ±10	XY -3642 ±10	ZXY 267 ±10		
Z6 -889 ±1	Z7 0 ±1	X2Y2 4764 ±1	ZX2Y2 5703 ±10	

Spin on Spin Off
Spin off 0 Hz

Read default shims Save1 Read1 Save2 Read2
Read shims from pars Save shims Read shims

Receiver gain 0 File

Autoshim
Start shim
Stop shim

#1 50.0 %
#2 10.0 %
#3 2.0 %

FID area 6.5
Rescale FID area 5

1. Z1 (+/- 10)
2. Z2

At least 30 min (1 cycle)
Poor shim -> Long time (3-4 cycle)

Lineshape sample

1H: CHCl₃ in Acetone-D₆

13C: Dioxane in Benzene-D₆

Routine shim

- 1) Spin off
- 2) Adjust Lock level 80
- 3) Z1-Z2-Z1
- 4) Z3-Z1-Z2-Z3-Z1-Z2
- 5) Z4-Z1-Z2-Z4-Z1-Z2
- 6) Turn off spin -> Repeat step 3), 4), 5)
- 7) Turn on spin -> 3)

Remove spinning sideband

- 1) Spin off
- 2) Adjust Lock level 80
- 3) X-Y-X-Y
- 4) X-ZX-X
- 5) Y-ZY-Y
- 6) X
- 7) XY-ZXY
- 8) X-Y-X-Y
- 9) Spin on
- 10) Z4 (asymmetry peak)
- 11) Z3-Z1-Z2

Typical interactions for axial shims:

- Z1 and all other axial shims, to some extent
- Z2 and Z1
- Z3 and Z1
- Z4 and Z2 (with large delta Z4s: Z4 and Z3)
- Z5 and both Z3 and Z1 (Z5 not available on 13-channel shim systems)

Table 42. Lineshape Effects and Their Associated Shims

<i>Lineshape Effect</i>	<i>Shims</i>
Split peak	Z4 and Z1
Asymmetry greater than half-way up	Z2
Asymmetric foot	Z4
Symmetric feet and or low broad base	Z5
Symmetrically broad base	Z3
Spinning sidebands	Low-order radials X1, Y1
Symmetric broad base	High-order radials X3, Y3, etc.

Tools > Standard Calibration Experiments > Shim Editor

The screenshot displays the Proshim software window, which is used for configuring shim methods. The interface is divided into several sections:

- Current method:** A dropdown menu shows "pfg_xyz_extended". Below it are buttons for "Start shim in background" (highlighted with a red box and a yellow '2'), "Stop shim", "Show shim log", and "Set as default on probe file".
- Method:** A table with columns Tol, Range, Steps, Delay, and Spin. It lists various shim methods like "pfg & lock1d", "lock1d", and "pfg & lock1d" with their respective parameters.
- FID-shim parameters:** A section for setting parameters for the current sample or using default values for a lineshape sample. Parameters include tpwr (53), pw (5.05), Acqtime (2.93601), d1 (2.5), gain (42), offset (699.7), and sw (11160.7).
- Manage shim method files:** A section for editing, showing, or deleting shim method files.

A green box highlights the "lock" and "lock1d" methods in the Method table, corresponding to the bulleted list provided below the image.

- lock—optimizes the lock shim variables as a group.
- lock1d—optimizes the lock shim variables independently in listed order.
- fid—optimizes the FID shim variables as a group.
- fid1d—optimizes the FID shim variables independently in listed order.
- Pfg – optimizes the shims using a z-gradient shim method.
- Gxyz – optimizes the shims using a 3D gradient shim method.

A white box with a green border contains the following text:

Lineshape sample
1H: CHCl₃ in Acetone-D₆
13C: Dioxane in Benzene-D₆

Create Gradient shim-map (Simple)

1H shimming: 10% H₂O in 90% D₂O
2H shimming: Doped 1% H₂O in 99% D₂O

The screenshot displays the Bruker QNP software interface with several key components highlighted for creating a gradient shim-map:

- Tools Menu (6):** The 'Tools' menu is open, and 'Set Up Gradient Shimming' is selected.
- Gradient Shim Setup (5):** The 'Acquire Trial Spectra' button is highlighted.
- Make Shimmap (4):** The 'Automake Shimmap' button is highlighted.
- Gradient Autoshim (2):** The 'Gradient Autoshim on Z' button is highlighted.
- Sequence Diagram (2):** The 'Sequence diagram' button is highlighted.
- Shimmap Plot (3):** A plot showing the shimmap results is highlighted.

The interface also shows a spectrum plot at the top right and a status bar at the bottom indicating 'Idle' and 'exp100: Acquisition complete'.

Create Gradient shim-map (Manually)

Exp: 100 Seq: gmapz Index: 1

1372.57

5 Type ds(1)
Set Window size (check height and Hz)

V_scale 249579.6 sp(Hz) -7194.27 wp(Hz) 15371.82 first 1 last 2 step 1

1

4

3

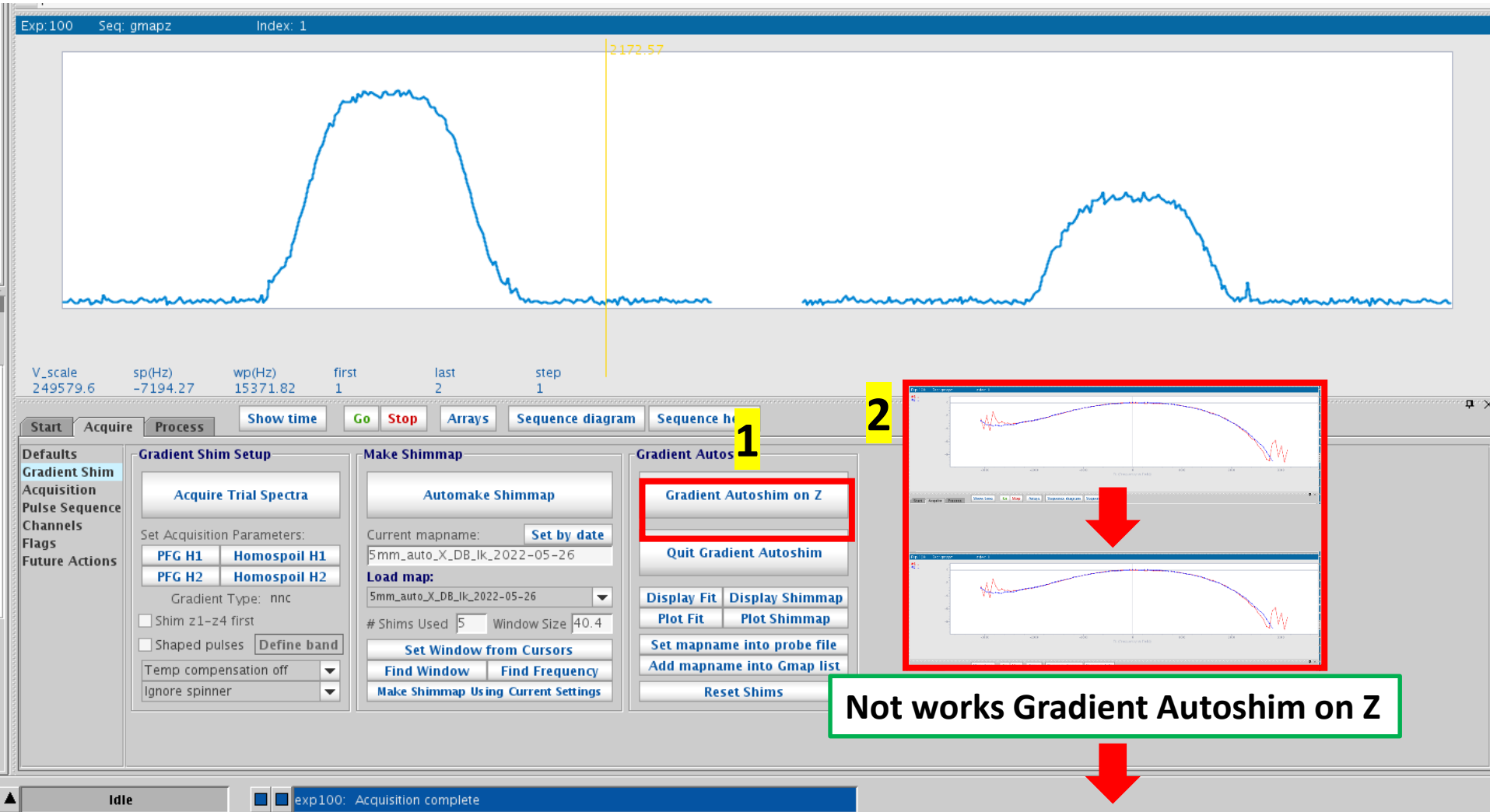
6

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exp100: Acquisition complete

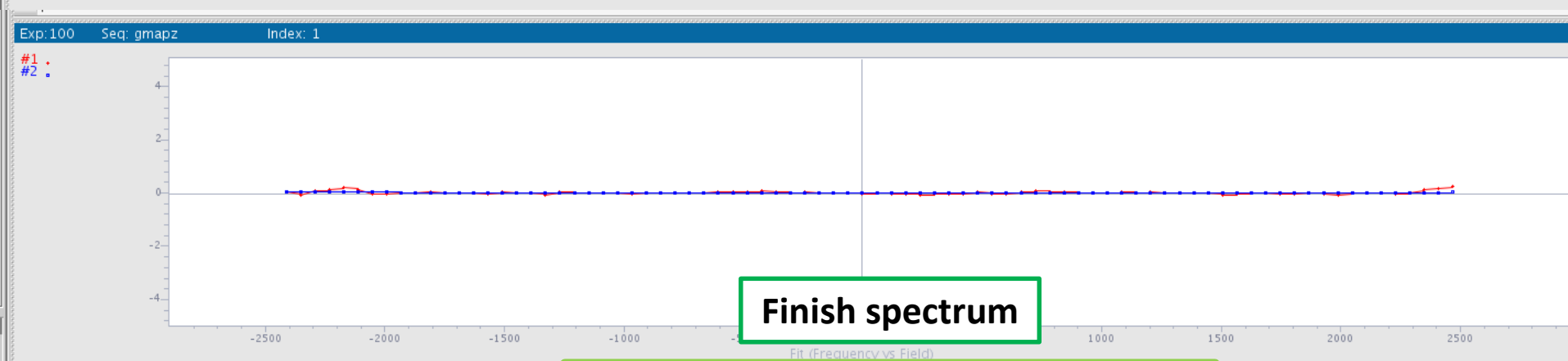
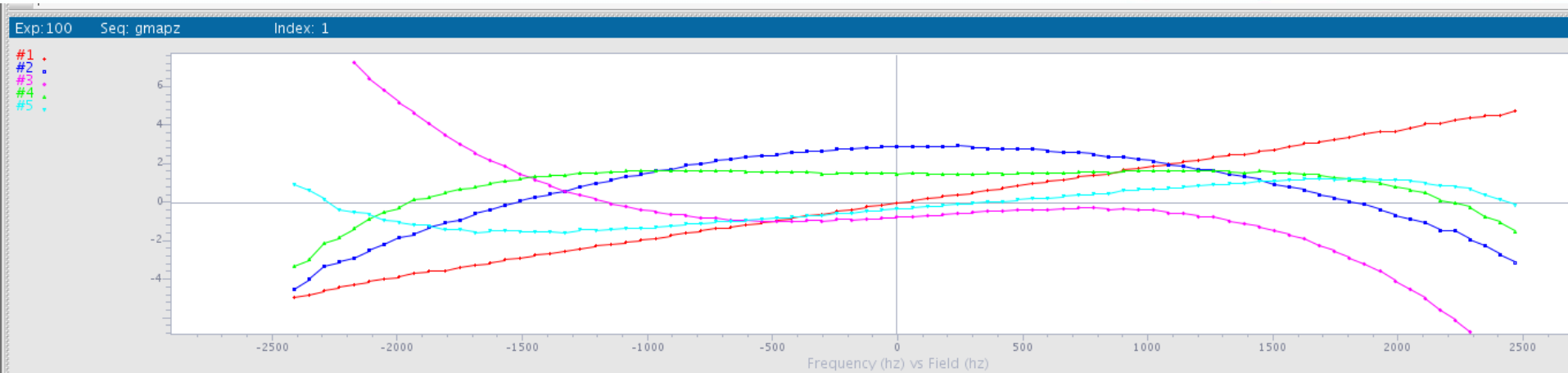
Create Gradient shim-map (Trouble shooting)



Not works Gradient Autoshim on Z

Try to use 3D shim or Shim editor

Finish shim-map



Finish spectrum

Start Acquire Process Show time Go Stop Arrays Seq

Defaults Gradient Shim Acquisition Pulse Sequence Channels Flags Future Actions

Gradient Shim Setup

Acquire Trial Spectra

Set Acquisition Parameters:

PFG H1 Homospoil H1

PFG H2 Homospoil H2

Gradient Type: nnc

Shim z1-z4 first

Make Shimmap

Automake Shimmap

Current mapname: 5mm_auto_X_DB_Ik_2022-06-09

Load map: 5mm_auto_X_DB_Ik_2022-06-09

Shims Used 5 Window Size 31.6

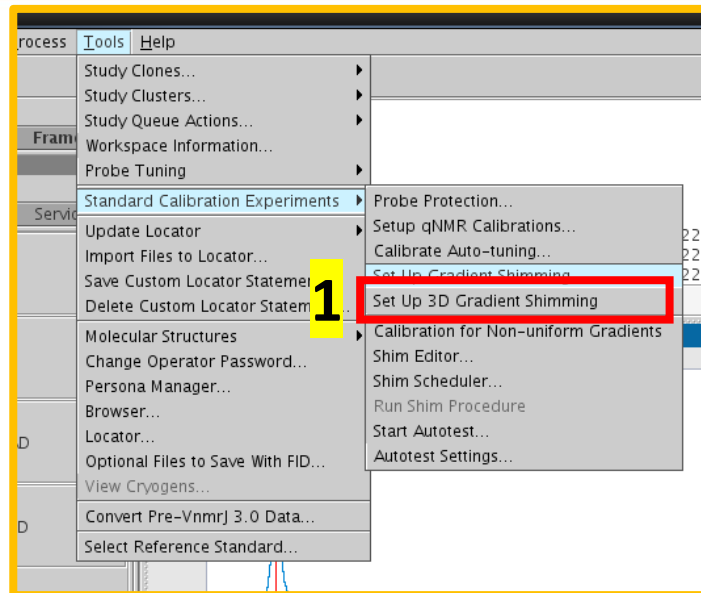
Display Fit Display Shimmap Plot Fit Plot Shimmap

Exp: 100 Seq: PROTON Index: 1

4.055
50% Inwidth: 2.09
95% Inwidth: 28.36
11% Inwidth: 63.80

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3D shim



At least 30 min (1 cycle)
Poor shim -> Try to use manual shim or shim editors

